Introduction to Bioinformatics Resources for NCI CCR Scientists

Bioinformatics Training and Education Program (BTEP)

https://btep.ccr.cancer.gov

Email: ncibtep@nih.gov

Slides and recording from this presentation (https://btep.ccr.cancer.gov/on-line-classes-2022)

We want to hear from you





Email: ncibtep@nih.gov

What kind of training is helpful to you?

Genome Analysis Unit (GAU) and BTEP Teams

Peter Fitzgerald

Carl McIntosh

Des Tillo

Amy Stonelake

Joe Wu

Alex Emmons

In this presentation, we will cover



Bioinformatics resources offered by the NCI CCR Bioinformatics Training and Education Program (BTEP)



Software purchased by OSTR for CCR researchers



NIH high performance computing Unix cluster Biowulf/Helix



NCI Cloud Resources



Resources offered by other NIH training programs

Topic: Resources on the BTEP website

Bioinformatics Training and Education Program



NIH Bioinformatics Calendar at https://btep.ccr.cancer.gov



Training – Online Classes 2022, Upcoming Classes, Class Archive



Resources – Bioinformatics FAQs, Video Archive, Class Documentation, New Resource Pages



Contact BTEP: ncibtep@nih.gov



NATIONAL CANCER INSTITUTE

Bioinformatics Training and Education Program

ncibtep@nih.gov

Home » Bioinformatics Training and Education Program

Bioinformatics Training and Education Program

The goal of the Bioinformatics Training and Education Program (BTEP), established by the Office of Science and Technology Resources (OSTR), is to increase the awareness and understanding of bioinformatics techniques and processes among CCR scientists, and to empower CCR scientists to perform a basic, informed set of analyses on their own behalf.

These training classes address the practical aspects of acquiring, representing, and analyzing complex biomedical data sets. Relevant theory and experimental design are also discussed. The goal is to provide both analytic recipes and to ensure better understanding of the theoretical and practical aspects of sound analytical technique.

REMOTE LEARNING

VIEW UPCOMING CLASSES

NIH Bioinformatics Calendar - Upcoming events

Hints on using the calendar, a grid view of the calendar and a view with past events is also available.



TOPIC FORMAT EVENT ORGANIZER PAST & FUTURE EVENTS

JULY

28

27 A COMPARATIVE ANALYSIS OF THE MOLECULAR **CHARACTERISTICS OF CANINE AND HUMAN GLIOMAS**

NCI IMAGING DATA COMMONS, PART OF THE CANCER RESEARCH **DATA COMMONS**

EVENTS AND RESOURCES



RESOURCES ~

Qlucore Bioinformatics Software for Next Gen Seg **Analysis**

Jul 13, 2022 | Announcement



Partek Flow: Bulk and Single Cell RNA-Seg Data Analysis

Iul 13, 2022 | Resources



Qiagen IPA Pathway Analysis Online Webinars in July

Jul 7, 2022 | Announcement



Learn Bioinformatics Skills with Dataquest and Coursera! Licenses are available.

May 31, 2022 | Resources



Updated Information on NIDAP bulk and single cell **RNA-Seq tutorials**

May 23, 2022 | Resources

EXTERNAL LINKS

Center for Cancer Research

Office of Science and Technology Resources

NIH Library Bioinformatics

JULY

27

JUL

A COMPARATIVE ANALYSIS OF THE MOLECULAR CHARACTERISTICS OF CANINE AND HUMAN GLIOMAS

28JUL

NCI IMAGING DATA COMMONS, PART OF THE CANCER RESEARCH DATA COMMONS

AUGUST

03

AUG

CHIP SEQUENCING DATA ANALYSIS

28

NCI IMAGING DATA COMMONS, PART OF THE CANCER RESEARCH DATA COMMONS



CALENDAR GOOGLECAL



EVENT DETAILS

This seminar series showcases research from different Cancer Moonshot initiatives that support the 10 recommendations of the Blue Ribbon Panel report. These presentations will inform the community about the progress of Cancer Moonshot–funded projects, provide outreach related to Cancer Moonshot projects, enhance discussions and collaborations related to Cancer Moonshot research, and promote the sharing of data from Cancer Moonshot initiatives.

Speaker: Andrey Fedoroy, Ph.D.Exit Disclain P.P. Brigham and Women's Hospital



REGISTER HERE

REGISTER

TIME

(Thursday) 12:00 pm - 1:00 pm

9

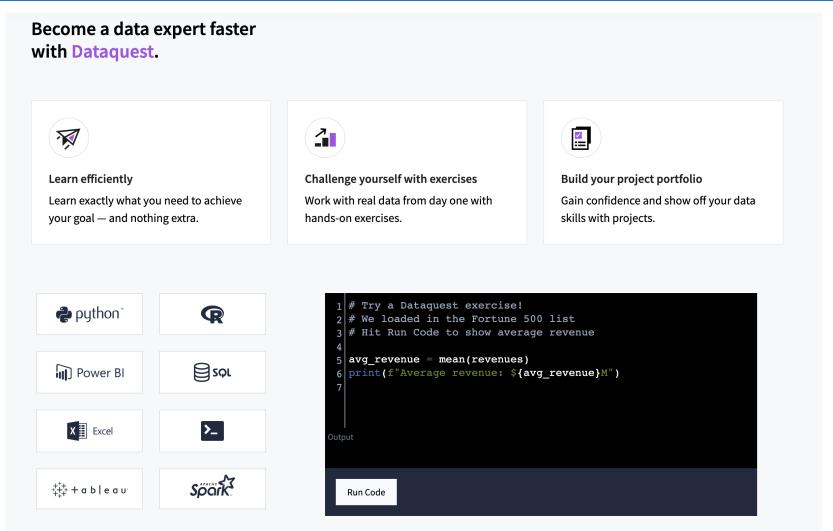
LOCATION

Online

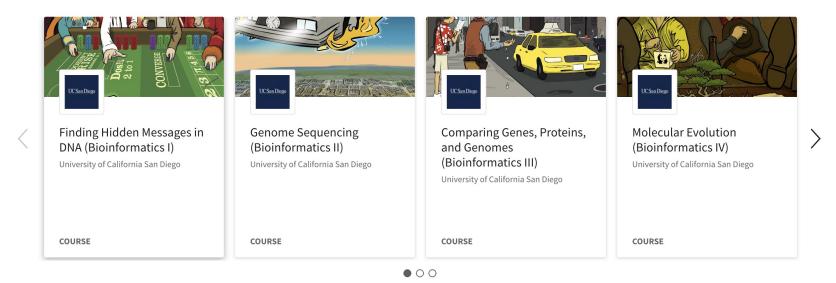
• ORGANIZER

Cancer Moonshot

Apply for a Dataquest license https://www.surveymonkey.com/r/2NPCBKT

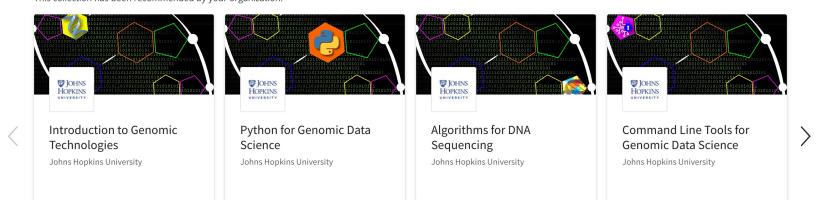


Apply for NIH Coursera license <u>here</u> Contact <u>ncibtep@nih.gov</u>



Genomic Data Science

This collection has been recommended by your organization.



Courses so far in 2022



Distinguished Speakers Seminar Series Rahul Satija, Melissa Haendel, Sarah Teichmann, Nicholas Navin



Topics in Bioinformatics – Microbiome Analysis with QIIME2, Variant Analysis



R classes – R basics, Visualization, and Data Wrangling



Software how-to — Bulk and Single Cell RNA-Seq, Pathway Analysis, Variant Analysis, Analyzing Publicly Available Data

BTEP Distinguished Speakers Seminar Series



Feb. 17, 1 PM.

Title: Integrated Analysis of Single Cell Data Across Technologies and Modalities

Rahul Satija, D.Phil., Core Faculty Member, New York Genome Center, Associate Professor of Biology, Center for Genomics and Systems Biology, New York University (NYU), Associate Faculty, Institute for Systems Genetics, NYU Langone Medical Center



April 21, 1 PM (Recording)

Title: Realizing Data Interoperability Across Basic Research, Clinical Care, and Patients

Melissa Haendel, Ph.D., Professor and Chief Research Informatics Officer, Marsico Chair in Data Science, University of Colorado, Anschutz Medical Campus

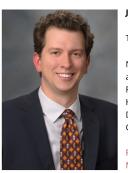


June 16, 1 PM.

Title: Mapping the Human Body One Cell at a Time

Sarah Teichmann, Ph.D., Fellow of the Acadamy of Medical Sciences (UK FMedSci), Fellow of the Royal Society (FRS), Wellcome Sanger Institute

WebEx recording: BTEP DSSS Sarah Teichmann-20220616 1704-1



July 14, 1 PM.

Title: Decoding Breast Cancer Progression with Single Cell Genomics

Nicholas Navin, Ph.D., Professor, MD Anderson Cancer Center, joint appointment in Dept of Bioinformatics
Faculty Member, The University of Texas, MD Anderson Cancer Center, UT Health Graduate School of Biomedical Sciences
Director of the CPRIT Single Cell Genomic Center
Co-Director, Advanced Technology Genomics Core at MD Anderson

Register Here Meeting Link



Sept 22, 1 PM

Christopher E. Mason, Ph.D., Professor, Department of Physiology and Biophysics Weill Cornell Medicine Director, WorldQuant Initiative for Quantitative Prediction

Register Here Meeting Link



October 27, 1 PM

Christina Curtis, Ph.D., M.Sc, Associate Professor of Medicine and Genetics, Stanford University School of Medicine, and Co-Director, Molecular Tumor Board, Stanford Cancer Institute

Register Here Meeting Link

BTEP Online Classes 2022

(https://btep.ccr.cancer.gov/on-line-classes-2022/)

Partek Flow: Bulk and Single Cell Gene Expression Visualization (May 18)

Recording link: https://cbiit.webex.com/cbiit/ldr.php? RCID=b5b1948aab3093124275d06fa55b08ae

Qlucore: Import and analyze public data from SRA, GEO and TCGA (May 11)

Recording link: https://cbiit.webex.com/cbiit/ldr.php? RCID=c8e8e8ff837caeb2d4d3839bc180b9bb

Training: Access GEO, SRA, ArrayExpress, TCGA, GTEx and more with Qiagen IPA Land Explorer (April 20)

Recording link: https://cbiit.webex.com/cbiit/ldr.php? RCID=d081980970fce4cb50dd20d3f4f3e172

Single Cell RNA-Seq Analysis with Partek Flow (April 13)

Recording Link:

https://cbiit.webex.com/cbiit/ldr.php%3FRCID%3D02b734d9f2b8466bf996ccc5d52d0c02

Qlucore: Pathway Analysis with Gene Set Enrichment Analysis (GSEA) (April 6)

Recording link: https://cbiit.webex.com/cbiit/ldr.php? RCID=8cfdd939b601f0402b312ba2f8e85262

Recommended Resources:

1. GSEA hands-on webinar_Qlucore.pdf

2. GSEA in Qlucore.pdf

Variant Analysis – Experimental Design, Best Practices, and Workflows (June 30)

Recording link:

https://cbiit.webex.com/recordingservice/sites/cbiit/recording/8cd6adf4dacc103a83be00505681c451

Presentation slides:

Variant analysis – presentation 1 Variant analysis – presentation 2

Chat history: chat history

Qlucore: Bulk RNA-Seq Data Analysis (June 29)

Recording link:

https://cbiit.webex.com/webappng/sites/cbiit/recording/c788382fd9e1103ab7f6005056818fce

Data Wrangling with R (June 7 – July 7)

Course Materials: https://btep.ccr.cancer.gov/docs/data-wrangle-with-r/

Lesson 1, June, 7th: Introduction to R, RStudio, and the Tidyverse

This will be a no coding introduction to R, RStudio, and the Tidyverse. In this lesson, we will review some of the advantages of using R for data analysis and will get you acquainted with the RStudio environment. The help session will be devoted to getting everyone connected to the course on DNAnexus.

Recording link: https://cbiit.webex.com/cbiit/ldr.php?RCID=5544470024885f1aa54c26fc5c9ff6cf

FAQs: Single Cell RNA-Seq, ChIP-Seq Analyses on the BTEP website



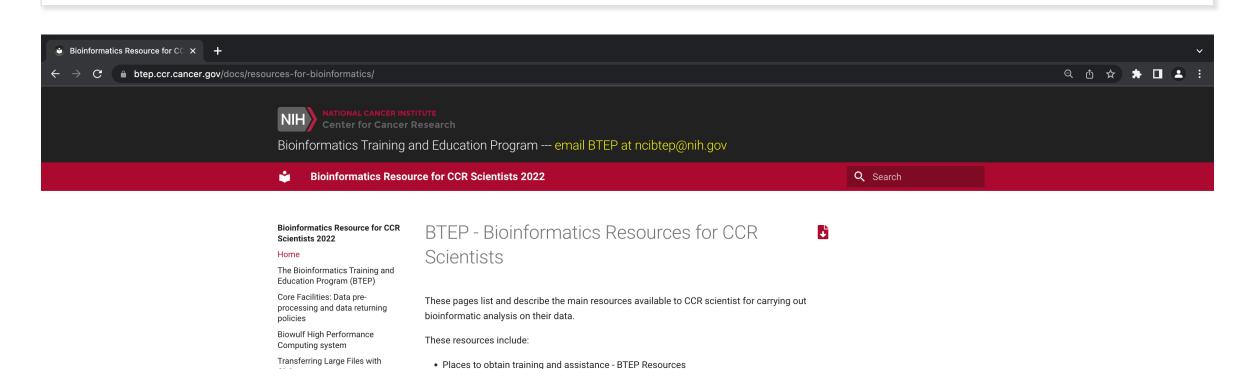


BTEP Resources Pages

Bioinformatic interest groups, listservs, and Slack channels

Go to the following website to check out the new BTEP bioinformatics resources pages :

https://btep.ccr.cancer.gov/docs/resources-for-bioinformatics/



Information about data delivered by the NCI sequencing facilities



Bioinformatics Training and Education Program --- email BTEP at ncibtep@nih.gov



Bioinformatics Resource for CCR Scientists 2022

Q Search

Bioinformatics Resource for CCR Scientists 2022

Home

The Bioinformatics Training and Education Program (BTEP)

Core Facilities: Data preprocessing and data returning policies

Biowulf High Performance Computing system

Transferring Large Files with Globus

Bioinformatic interest groups, listservs, and Slack channels

More Training Opportunities

>

Self Learning Platforms

Select Software By Topic

Non-commerical Software

Commercial Software

Core Facilities: Data pre-processing and data returning policies



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Core Facilities

Understanding QA/QC reports

fastqc

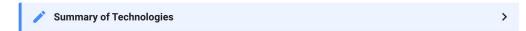
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Core Facilities

There are a number of core facilities available to NCI researchers. See more information from the Office of Science and Technology Resources.

We most commonly see data from the following cores:

- 1. CCR Sequencing Facility (CCR-SF) located at the ATRF in Frederick, MD. This core is dedicated to high throughput sequencing.
 - For large scale projects and production ready projects (compare with NCI CCR Genomics Core)



- 2. NCI CCR Single Cell Analysis Facility (SCAF) located on the NIH Bethesda main campus and provides advanced single-cell genomics technologies.
 - Primarily for CCR researchers on the Bethesda campus.



Bioinformatics Training and Education Program --- email BTEP at ncibtep@nih.gov



Bioinformatics Resource for CCR Scientists 2022



Bioinformatics Resource for CCR Scientists 2022

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Getting Started with Biowulf

Biowulf is the NIH high performance computing cluster. It is a linux computing cluster with greater than 105,000 processors. The NIH HPC systems also house "hundreds of scientific programs, packages and databases" (https://hpc.nih.gov/apps/).

Bioinformatic processes often require a lot of memory and computational time, which is limited on individual (local) computers. For bioinformatics tasks that require a lot of memory or can be run in parallel to reduce the time to completion, consider performing such tasks on Biowulf. To obtain a Biowulf account, see the Biowulf help pages. A Biowulf account is accessible to all NIH employees and contractors listed in the NIH Enterprise Directory for a nominal fee of \$35 a month.

Working on the NIH High Performance Unix Cluster Biowulf

Logging into Biowulf from MacOS

Find the program "Terminal" on your machine, and enter the following statement at the prompt:

ssh username@biowulf.nih.gov



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Working on the NIH High Performance Unix Cluster Biowulf

Logging into Biowulf from MacOS

Logging into Biowulf from Windows 10 OS

Working on Biowulf - two things you should always do.

Being a good citizen on Biowulf

Running Interactive Jobs

Batch Jobs

Swarm-ing on Biowulf



Bioinformatics Training and Education Program --- email BTEP at ncibtep@nih.gov



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NIH Integrated Data Analysis Platform (NIDAP)



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Description

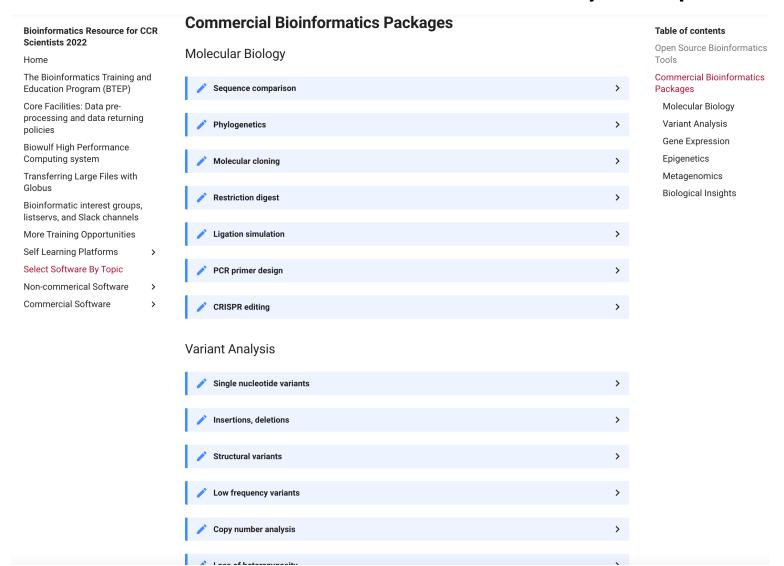
Description

NIDAP (NIH Integrated Data Analysis Platform) is an innovative, cloud-based, collaborative data aggregation and analysis platform that hosts user-friendly bioinformatics workflows and component analysis and visualization tools developed by the NCI developer community based on open source tools and makes them immediately available to biologist end-users across the Institute. --- (https://ccbr.ccr.cancer.gov/education-training/nidap-workflows/)

It is a free resource to NCI researchers that can be used for bulk and single cell RNA-Seq analyses. The platform is a graphic user interface (GUI) that does not require users to read or write code. Free training is offered monthly so that researchers can learn to use the workflows on the platform and understand the results.

For more information, including how to access the platform, and current training dates, please see: https://btep.ccr.cancer.gov/nidap_announce/.

BTEP – Select Software by Topic



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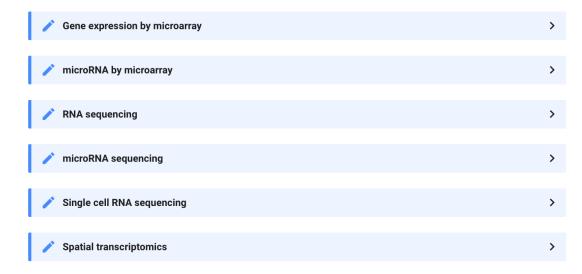
Self Learning Platforms

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Commercial Software

Gene Expression



Epigenetics

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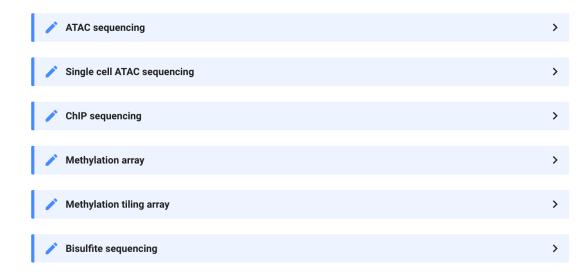


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Open Source Bioinformatics

Commercial Bioinformatics Packages

Molecular Biology

Variant Analysis

Gene Expression

Epigenetics

Metagenomics

Biological Insights

Upcoming courses of interest

Bioinformatics for Beginners

- Unix/ Biowulf
- Bulk RNA-Seq Data Analysis

Distinguished Speakers Seminar Series

- Christopher Mason
- Christina Curtis

Topics in bioinformatics

- Bulk RNA-Seq
- Single Cell RNA-Seq
- ChIP-Seq
- Microbiome analysis

Next topic: Data Analysis Options Licensed Software

NIH HPC BIOWULF

How should you analyze your data?



Using proprietary, point-and-click software purchased for NCI CCR scientists by Office of Science and Technology Resources (OSTR)

May not always be in an environment where these are available

Partek Flow, and Partek Genomics Suite, Qiagen Ingenuity Pathway Analysis, Qlucore Omics Explorer



Learn open source tools, step-by-step

Lots to learn (Unix, R, Python, HPC Biowulf/Helix)
Knowledge transfers outside of NIH
GATK, GSEA, BWA, RSEM, STAR, Salmon

Office of Science and Technology Resources (OSTR)







MAKES LICENSES TO SOFTWARE AVAILABLE TO ALL NCI CCR RESEARCHERS (SOME ARE ALSO AVAILABLE TO ALL NCI RESEARCHERS, NOT JUST CCR)



NIH LIBRARY OFFERS SOME OF THE SAME LICENSES FOR ALL OF NIH



TYPES OF DATA ANALYSIS: NEXT GEN SEQUENCING, STATISTICS, PATHWAY

NCI CCR OSTR licensed software

Partek Flow and Partek Genomics Suite

Qiagen Ingenuity Pathway Analysis and OmicSoft Land Explorer

Qlucore Omics Explorer

Qiagen CLC Genomics Workbench

SnapGene

LaserGene

Geneious (Prime)

Graph Pad Prism

Molecular Biology Software

Geneious (Prime)

SnapGene

LaserGene

Partek Genomics Suite

CLC Genomics Workbench

Partek Flow for Single Cell RNA-Seq Analysis

Focus on:

Qiagen IPA for Pathway Analysis and 'omics data access

Partek Flow Applications

Single Cell RNA-Seq (and spatial transcriptomics)

Gene Expression (RNA-Seq, qPCR, microarray data)

Variant Detection

CNV Analysis

Metagenomics (microbial genomes)

Methylation

ChIP-Seq

Non-coding RNA Analysis

Multiomic Analysis

How to Learn Partek Flow

Extensive library of webinars and tutorials on Partek.com

BTEP-sponsored training sessions, recordings and resource pages

Partek Flow: Single Cell RNA-Seq Data Analysis

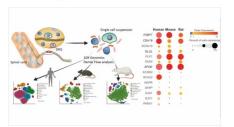
Start with fastq or count matrix (10x Genomics)

- Filtering (exclude barcodes, unique molecular identifiers)
- Drop out low quality cells and uninformative genes
- Interactive QA/QC plots (reads, genes and %mitochondrial reads/cell)

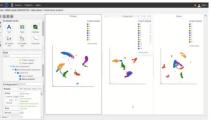
Can do:

- Trajectory analysis
- Differential gene expression analysis
- Tissue transcriptomics

Our Single Cell Webinar Series



Satellite Glial Cells Role in Neural Repair

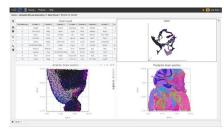


Single Cell Multiomics with COVID-19

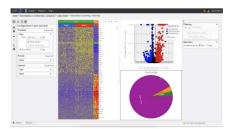
Data



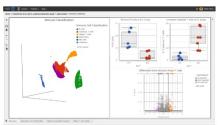
Multiomics Analysis



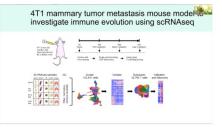
Spatial Transcriptomics Analysis



Partek Flow - New Single Cell and Bulk RNA-Seq Features



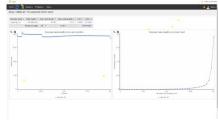
Single Cell RNA-Seq Analysis



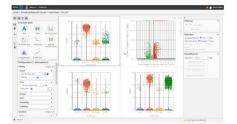
Evolution of Mouse Immune Response

During Mammary Tumor Progression

and Metastasis



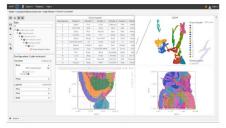
Understanding Data Formats and Preprocessing



Visualizing Single Cell Data with Figures



Differential Gene Expression Analysis



10x Visium Spatial Gene Expression

Data



Single Cell Analysis - inDrop System and Partek Flow

Qiagen Ingenuity Pathway Analysis (IPA) and OmicSoft Land Explorer Licenses recently purchased for CCR scientists to access Qiagen OmicSoft Land Explorer which contains data from GEO, SRA, ArrayExpress, TCGA, GTEx and more

In addition to Qiagen IPA licenses for Pathway Analysis

Qiagen Ingenuity Pathway Analysis

QIAGEN

Understand complex 'omics data to accelerate your research

Discover why QIAGEN Ingenuity Pathway Analysis (IPA) is the leading pathway analysis application among the life science research community and is cited in tens of thousands of articles for the analysis, integration and interpretation of data derived from 'omics experiments. Such experiments include RNA-seq, small RNA-seq, metabolomics, proteomics, microarrays including miRNA and SNP, and small-scale experiments. With QIAGEN IPA you can predict downstream effects and identify new targets or candidate biomarkers. QIAGEN Ingenuity Pathway Analysis helps you perform insightful data analysis and interpretation to understand your experimental results within the context of various biological systems.



Qiagen OmicSoft Land Explorer

Contextualize your findings with a massive collection of 'omics data

QIAGEN IPA now offers contextually relevant links to QIAGEN OmicSoft Land Explorer, a database of curated disease 'omics data with over 500,000 samples. With this new premium tier of IPA, you can explore 'omics data for individual genes as well as expression correlation across multiple genes with robust visualizations. Jump from a gene of interest in QIAGEN IPA to discover its tissue or cell expression. Explore the diseases and treatment contexts in which it is up-or-down-regulated. Visualize how mutations correlate with changes in expression, the effect of mutations on clinical outcomes and much more. Access to OmicSoft Land Explorer through IPA requires additional licensing.

Further details on the integration of QIAGEN IPA with QIAGEN OmicSoft Land Explorer can be found here.



Topic: NIH HPC Biowulf

Biowulf (highperformance cluster)



hpc.nih.gov



Thousands of analysis tools (modules) maintained by staff



Scientific reference databases



Next-gen sequencing, computational chemistry, math, statistics, image analysis



User guides and training classes



Monthly Zoom-In Consults see BTEP NIH Calendar

Why you should get to know Biowulf



BIOWULF IS THE HIGH PERFORMANCE CLUSTER (HPC) AT NIH.



IT CAN HOLD A LOT MORE DATA THAN YOUR PERSONAL COMPUTER.



IT HAS MUCH MORE COMPUTE RESOURCES THAN YOUR PERSONAL COMPUTER.



IT CAN HELP YOU ANALYZE "BIG DATA".



IT IS AVAILABLE TO ALL NCI CCR RESEARCHERS (ALL NIH RESEARCHERS).

Connecting to Biowulf

You can log onto Biowulf from MacOS or Windows PC

You'll need to learn some Unix/command-line/shell

Several different ways to use compute resources (batch, swarm)

How to learn more about Biowulf



BTEP Biowulf Beginner Classes



HPC Biowulf Monthly Zoom-In Consults (check BTEP calendar)



hpc.nih.gov

Data Transfer and Sharing on HPC Biowulf

Globus can transfer very large data files between your machine and Biowulf

You can mount a Biowulf drive on your local machine

Transfer to and from Cloud resources

Share data with collaborators (inside and outside of NIH)

(https://hpc.nih.gov/docs/transfer.html)

NCI and NIAID Workflows on Biowulf

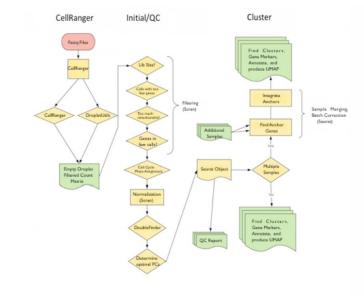
CCBR Pipeliner – bulk and single cell RNA-Seq and ChIP-Seq analysis workflows on NIH HPC Biowulf from the CCR Collaborative Bioinformatics Resource (https://github.com/CCBR)

NIAID Collective Bioinformatics Resource (NCBR) OpenOmics/genome-seek: Clinical Whole Genome Sequencing Pipeline (https://github.com/OpenOmics/genome-seek)

CCBR Pipeliner and Software

- Whole Exome and Genome pipelines
- Single Cell RNA-Seq pipeline
- RNA-Seq Pipeline
- ChIP-Seq Pipeline

Single Cell RNA-Seq Pipeline



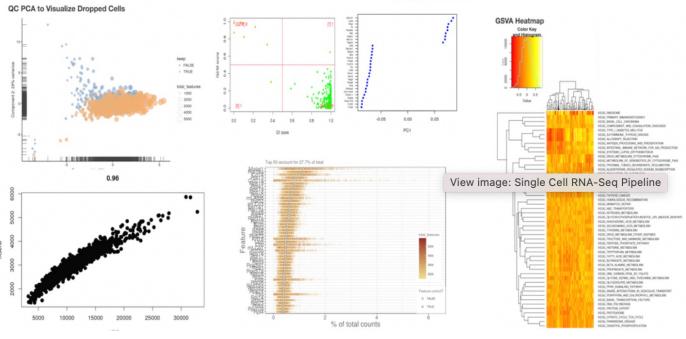
Starting points

- 10X genomics fastq
- 10X genomics count matrix

Data Filtering and QC

Downstream analysis

- k-means clustering
- PCA
- tSNE plot
- marker gene lists



Next topic: Cloud Resources

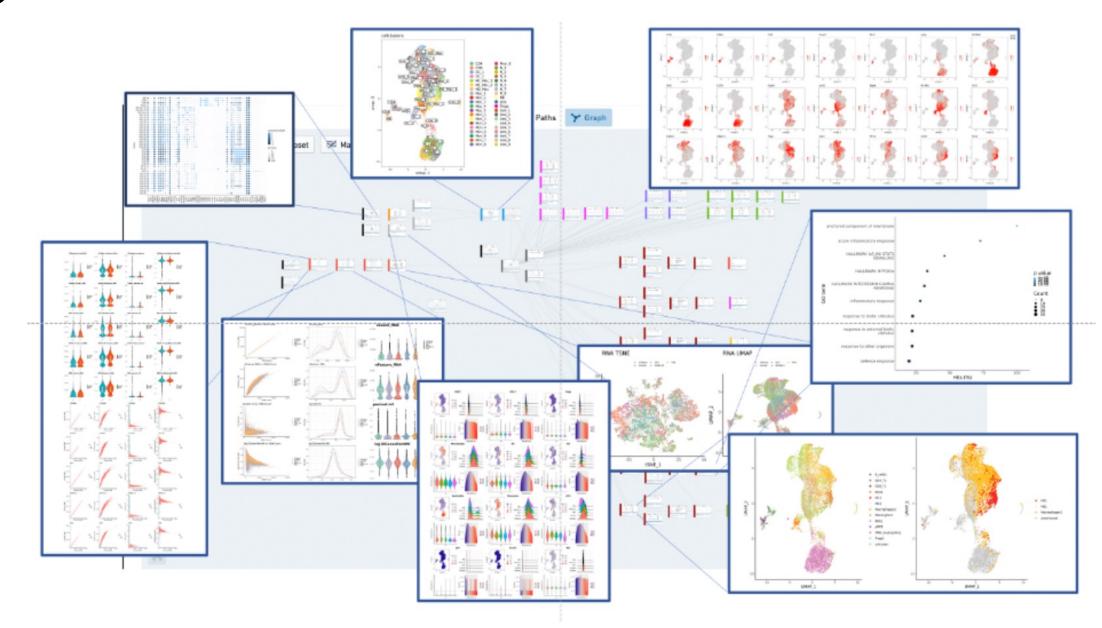
Cloud Resources

NIDAP – NIH Integrated Data Analysis Platform –bulk and single-cell RNA Seq Analysis Workflows on Palantir Foundry from the CCR Collaborative Bioinformatics Resource (https://ccbr.ccr.cancer.gov/education-training/nidap-workflows/)

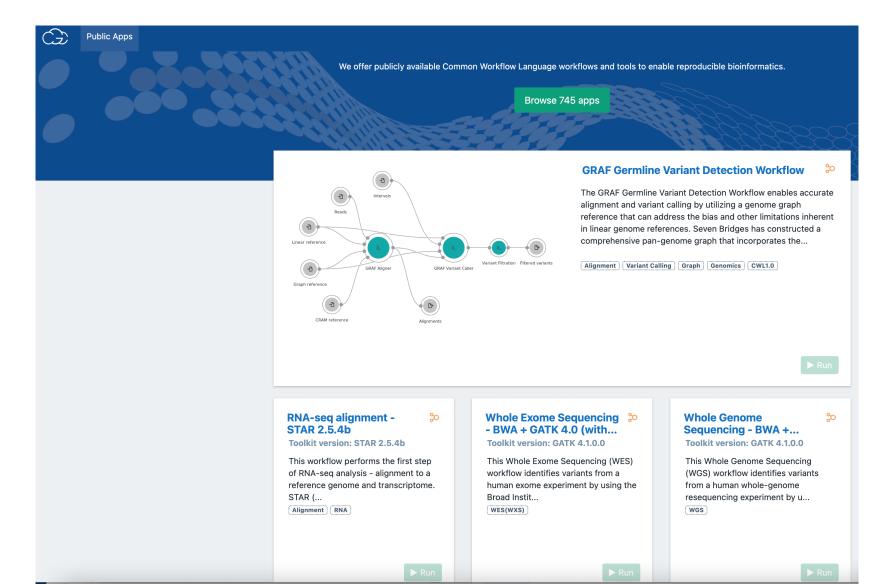
NCI Cancer Research Data Commons (CBIIT) including Cancer Genomics Cloud powered by Seven Bridges (https://datacommons.cancer.gov/analytical-resource/seven-bridges-cancer-genomics-cloud)

DNAnexus pilot AWS cloud access with both user-friendly GUI and command line interfaces (send email to ncibtep@nih.gov)

NIDAP



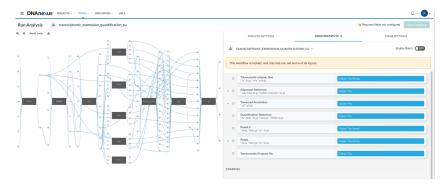
Cancer Genomics Cloud powered by Seven Bridges





The power of the Cloud via a simple Web-based Interface

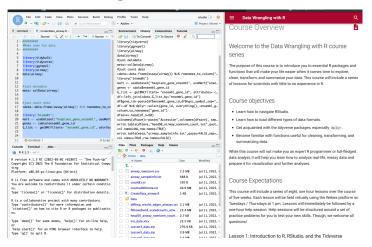
Pre-built workflows - RNA-Seq Expression Workflow



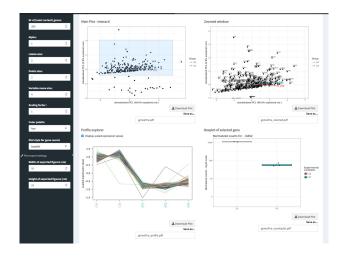
Custom Solutions - Interactive Data Analysis



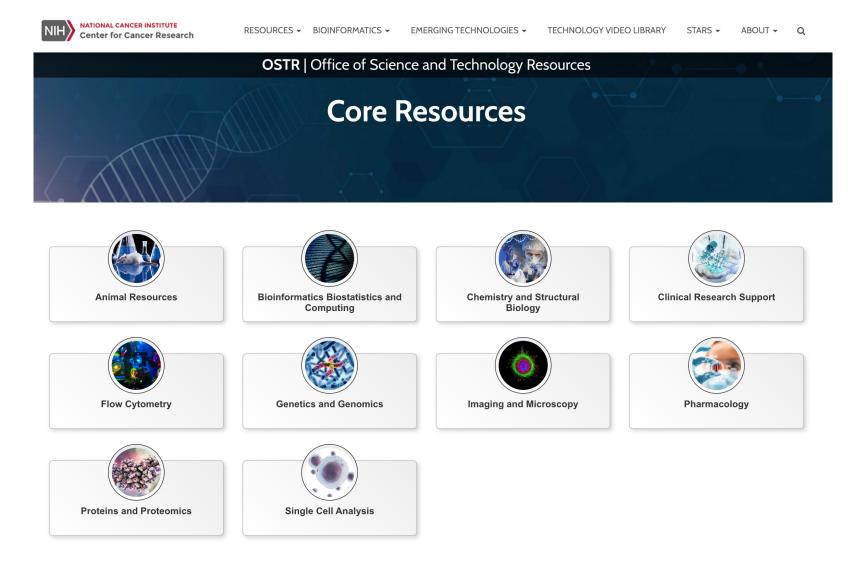
Training Environments - Unix and R



Hosted R Shiny Apps – PCA Explorer



Next topic: Core Resources



Focus on: Sequencing Cores

CCR Sequencing Facility (CCR-SF)(ATRF in Frederick)

- For large scale projects*
- Short read and long read technologies
- Single cell -omics
- Optical mapping with Bionano

NCI CCR Single Cell Analysis Facility (SCAF) (Building 41)

 Advanced single cell genomics for researchers on the NIH Bethesda main campus

NCI CCR Genomics Core (Building 37)

- For small scale projects*
- Example technologies: short read NGS, long read Oxford Nanopore MinION, Sanger sequencing, digital droplet PCR, etc.

Other Bioinformatics Resources and Training

All training events are available on the BTEP NIH Bioinformatics Calendar

List serv at <u>list.nih.gov</u>

NIH Library offers training classes in software and NGS analyses

Center for Biomedical Informatics and Information Technology (CBIIT)

CBIIT NCI Data Science Learning Exchange (machine learning, python)

Bioinformatics List Serves at NIH

Welcome to NIH LISTSERV list.nih.gov

BIOINFORMATICS-SIG-L (NIH Bioinformatics Special Interest Group)

NIH-DATASCIENCE-L (Data Science at NIH)

SINGLE-CELL-GENOMICS-L (Single-Cell Genomics)

Thank you for your support!

Office of Science and Technology Resources (OSTR)

Dave Goldstein Mariam Malik

CCR and NIAID Collaborative Bioinformatics Resources

Thank you for helping us by providing expert knowledge about bioinformatics tools and resources

We couldn't do the training we do without your support

Maggie Cam (CCBR Lead)

Parthav Jailwala (CCBR Bioinformatics Manager)

Justin Lack (NCBR Lead)

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Genome Analysis Unit (GAU) and BTEP Teams

Peter Fitzgerald

Carl McIntosh

Des Tillo

Amy Stonelake

Joe Wu

Alex Emmons

Slides and recording from this presentation (https://btep.ccr.cancer.gov/on-line-classes-2022)

We want to hear from you





Email: ncibtep@nih.gov

What kind of training is helpful to you?